LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100501.D
Acq On : 13 Nov 2017 14:35
Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	28	rVB2	21727	50609	2.67%	0.279%
2	5.116	510	515	525	rVB	264108	325658	17.20%	1.793%
3	5.510	576	582	585	rBV	1795422	1744846	92.18%	9.606%
4	6.516	747	753	757	rBV	1729082	1828632	96.60%	10.067%
5	6.657	772	777	781	rBV	1891006	1830007	96.68%	10.075%
6	6.893	813	817	820	rVB	592205	532944	28.15%	2.934%
7	7.045	839	843	846	rBV	1610461	1401970	74.06%	7.718%
8	7.451	907	912	915	rBV	1222642	1103119	58.28%	6.073%
9	8.169	1031	1034	1037	rBV	796146	660596	34.90%	3.637%
10	8.586	1102	1105	1107	rBV	26008	22093	1.17%	0.122%
11	9.245	1212	1217	1220	rBV	2279755	1892915	100.00%	10.421%
12	9.322	1225	1230	1232	rBV2	33490	33442	1.77%	0.184%
13	9.633	1280	1283	1287	rBV	211000	167378	8.84%	0.921%
14	9.851	1312	1320	1324	rVB2	24710	38916	2.06%	0.214%
15	9.928	1328	1333	1336	rVV	811582	707555	37.38%	3.895%
16	9.957	1336	1338	1340	rVB	40257	28415	1.50%	0.156%
17	10.122	1361	1366	1370	rVB4	22234	31457	1.66%	0.173%
18	10.239	1381	1386	1388	rBV4	28141	36015	1.90%	0.198%
19	10.298	1393	1396	1399	rVV	153027	127933	6.76%	0.704%
20	10.345	1403	1404	1408	rVB	33260	24717	1.31%	0.136%
21	10.569	1438	1442	1447	rVB3	19771	31269	1.65%	0.172%
22	10.633	1447	1453	1457	rBV2	30112	38106	2.01%	0.210%
23	10.710	1461	1466	1470	rBV	1118847	1068320	56.44%	5.881%
24	10.833	1482	1487	1490	rVB2	48808	60126	3.18%	0.331%
25	11.269	1555	1561	1563	rBV2	36781	41559	2.20%	0.229%
26	11.298	1563	1566	1574	rVB4	29741	42138	2.23%	0.232%
27	11.410	1581	1585	1588	rBV	769455	645344	34.09%	3.553%
28	11.433	1588	1589	1592	rVB	127830	69186	3.65%	0.381%
29	11.516	1600	1603	1606	rBV2	19921	25855	1.37%	0.142%
30	11.692	1631	1633	1636	rVB2	23796	22226	1.17%	0.122%
31	11.739	1636	1641	1647	rVB7	18400	29555	1.56%	0.163%
32	11.927	1667	1673	1679	rBV2	185023	229344	12.12%	1.263%
33	12.022	1686	1689	1691	rBV2	33974	33177	1.75%	0.183%
34	12.104	1700	1703	1707	rBV2	33745	31501	1.66%	0.173%

LSC Area Percent Report

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Data File : BF100501.D
Acq On : 13 Nov 2017 14:35
Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.204	1717	1720	1722	rBV	27007	25161	1.33%	0.139%
36	12.386	1748	1751	1753	rBV2	22699	24564	1.30%	0.135%
37	12.463	1761	1764	1767	rBV	50054	39740	2.10%	0.219%
38	12.492	1767	1769	1772	rVB2	44300	38694	2.04%	0.213%
39	12.551	1776	1779	1783	rBV4	20959	30049	1.59%	0.165%
40	12.622	1789	1791	1796	rBV	170787	161790	8.55%	0.891%
41	12.710	1803	1806	1811	rBV3	78556	85232	4.50%	0.469%
42	12.851	1827	1830	1836	rVB	151702	146448	7.74%	0.806%
43	12.992	1850	1854	1858	rVB	1411351	1259448	66.53%	6.934%
44	13.063	1863	1866	1869	rBV4	30211	40356	2.13%	0.222%
45	13.174	1883	1885	1888	rVB	34161	32067	1.69%	0.177%
46	13.216	1890	1892	1895	rBV4	25810	23307	1.23%	0.128%
47	13.880	2002	2005	2010	rBV2	115138	122589	6.48%	0.675%
48	14.051	2029	2034	2036	rBV	613546	608496	32.15%	3.350%
49	14.074	2036	2038	2040	rVB	68530	50606	2.67%	0.279%
50	15.527	2281	2285	2296	rVB	343244	519076	27.42%	2.858%

Sum of corrected areas: 18164546

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
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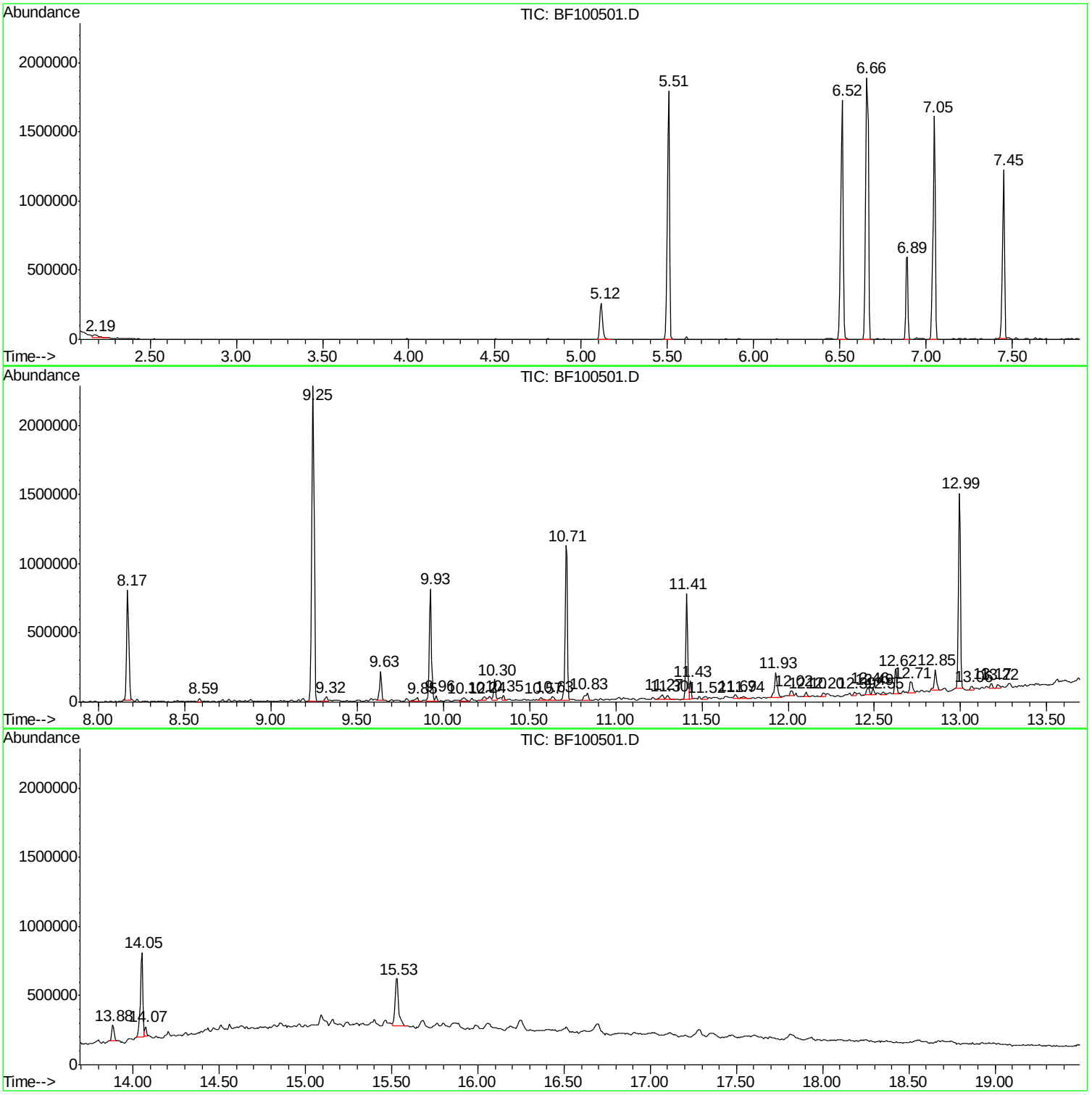
Acq On : 13 Nov 2017 14:35
Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100501.D
Acq On : 13 Nov 2017 14:35
Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

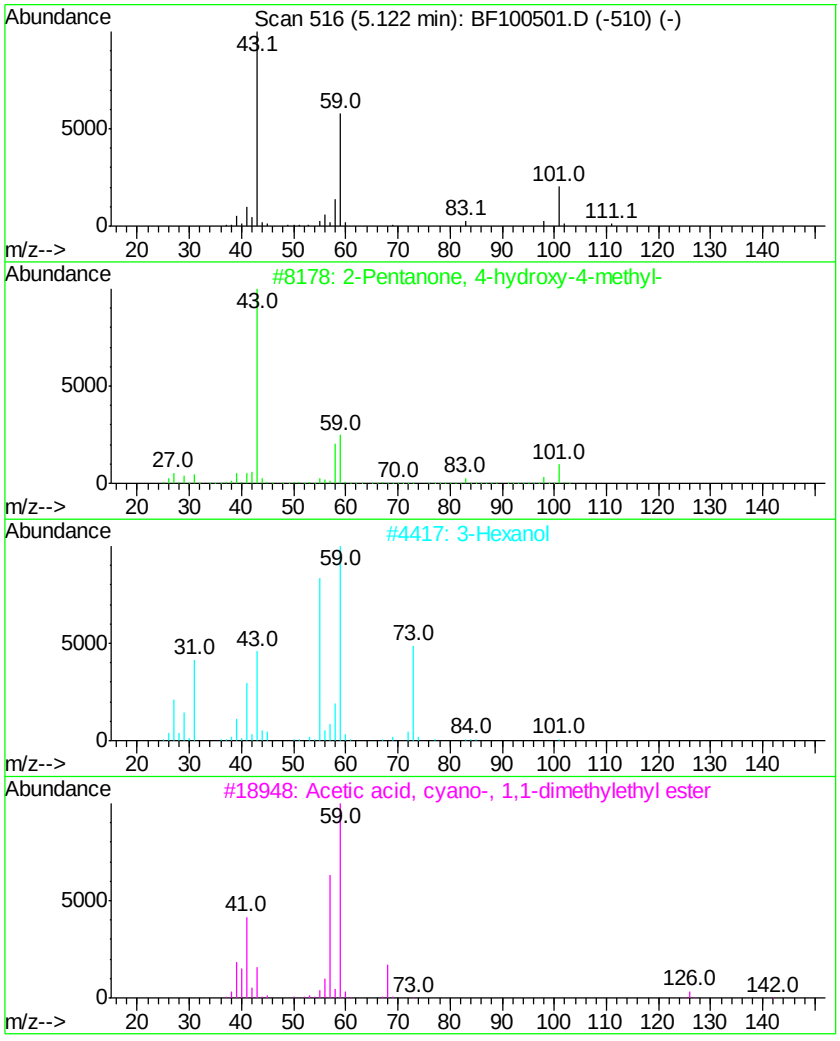
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

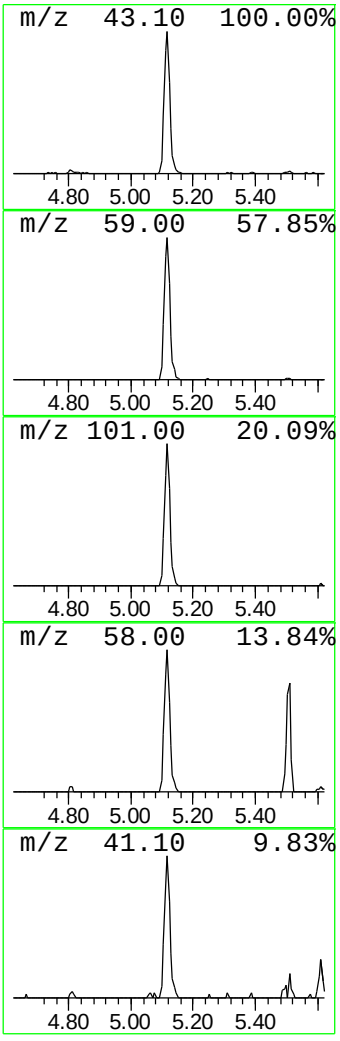
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.22 ng	325658	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100501.D
Acq On : 13 Nov 2017 14:35
Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

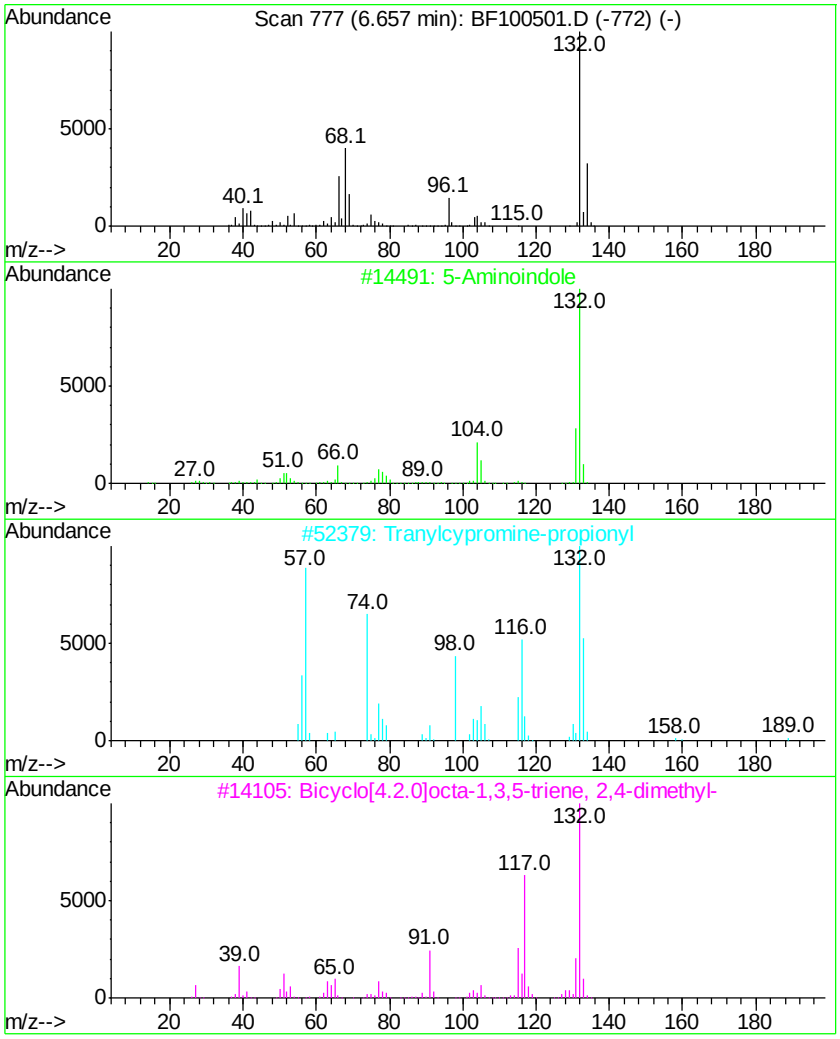
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

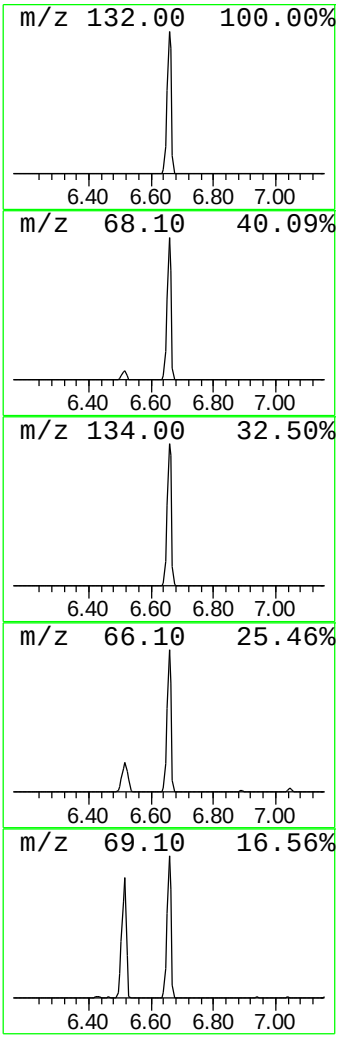
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.68 ng	1830010	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100501.D
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Operator : SJ/JU
Sample : I6399-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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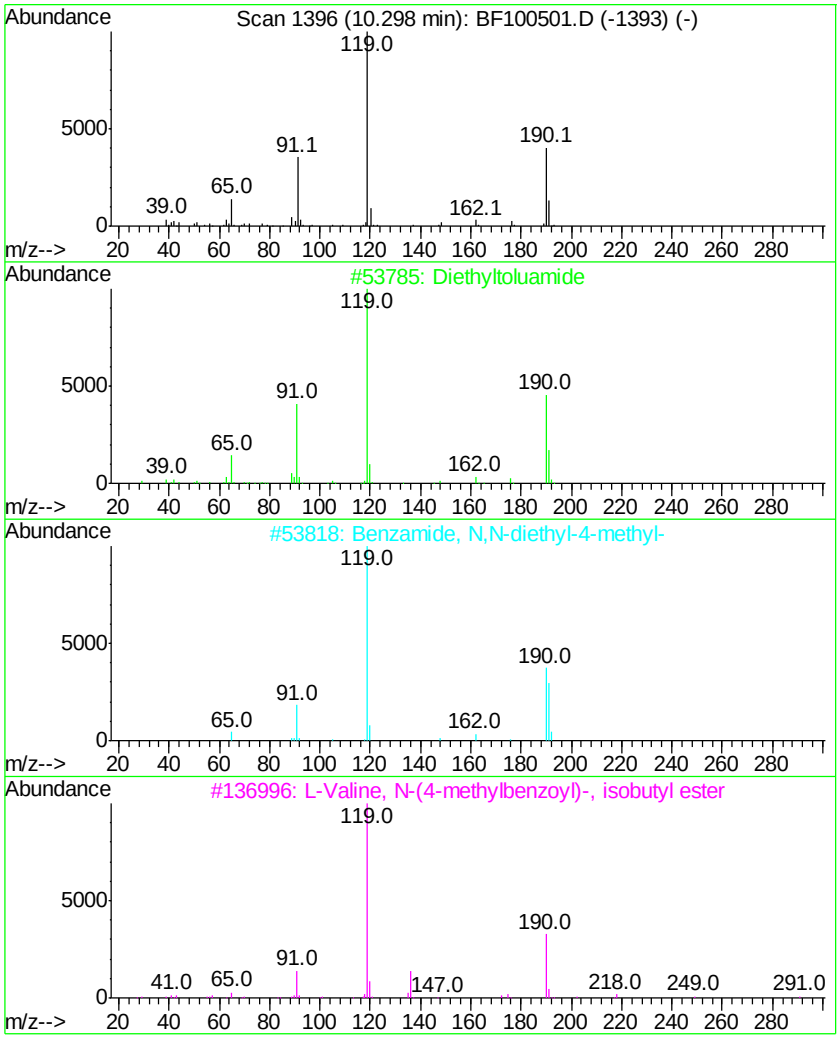
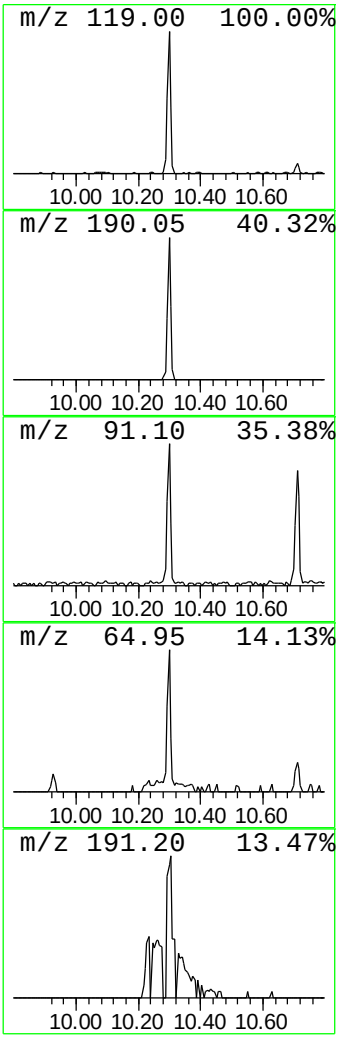
Peak Number 4 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	3.62 ng	127933	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	78
3	L-Valine, N-(4-methylbenzoyl)-, ...	291	C17H25NO3	1000346-63-9	72
4	L-Valine, N-(4-methylbenzoyl)-, ...	291	C17H25NO3	1000346-64-0	72
5	4'-Methylbutyrophenone	162	C11H14O	004160-52-5	50





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

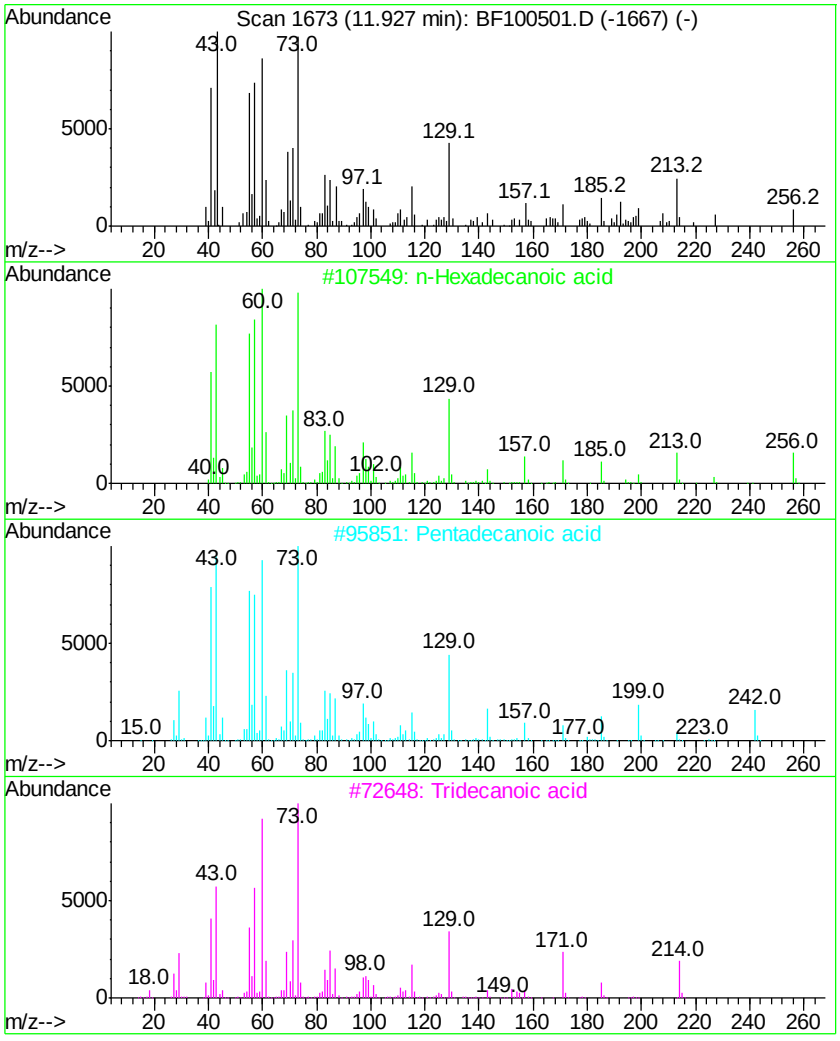
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

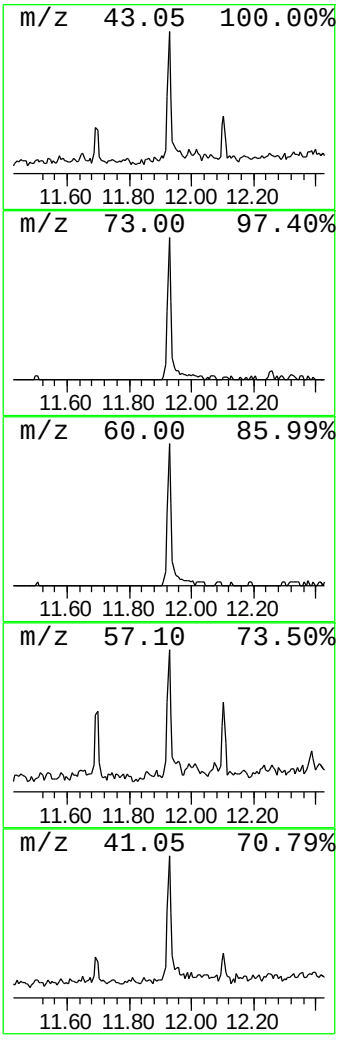
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	7.11 ng	229344	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

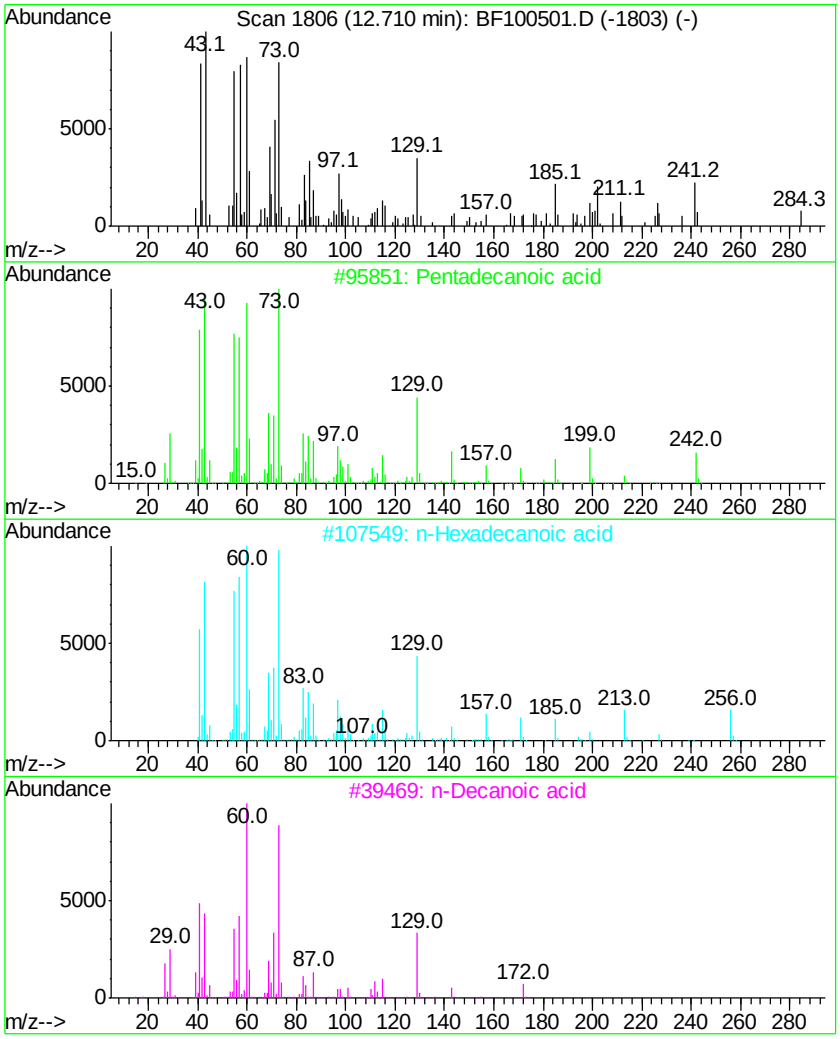
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

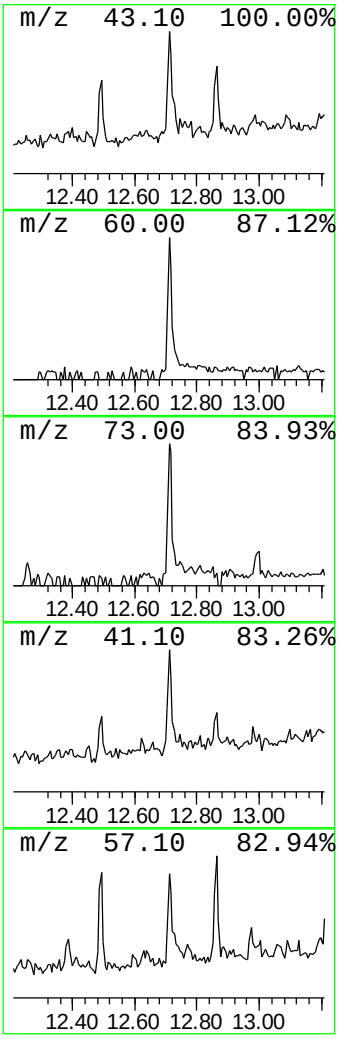
****

Peak Number 6 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.64 ng	85232	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	55
4	Undecanoic acid	186	C11H22O2	000112-37-8	55
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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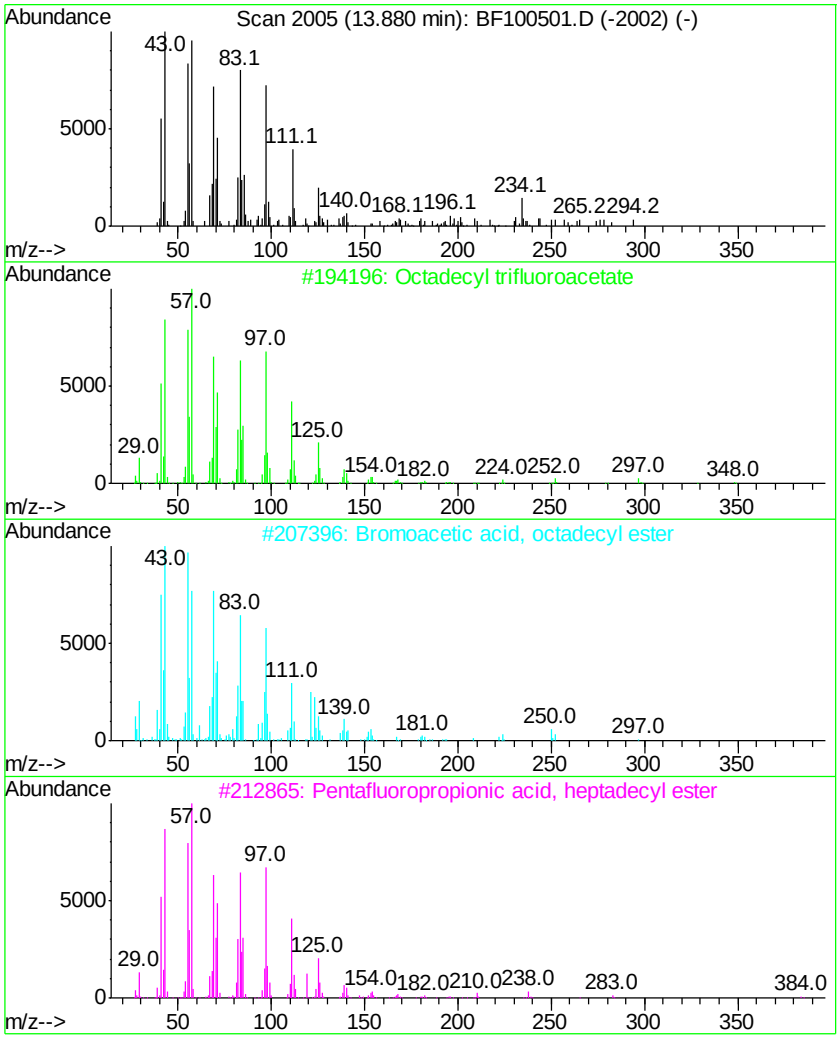
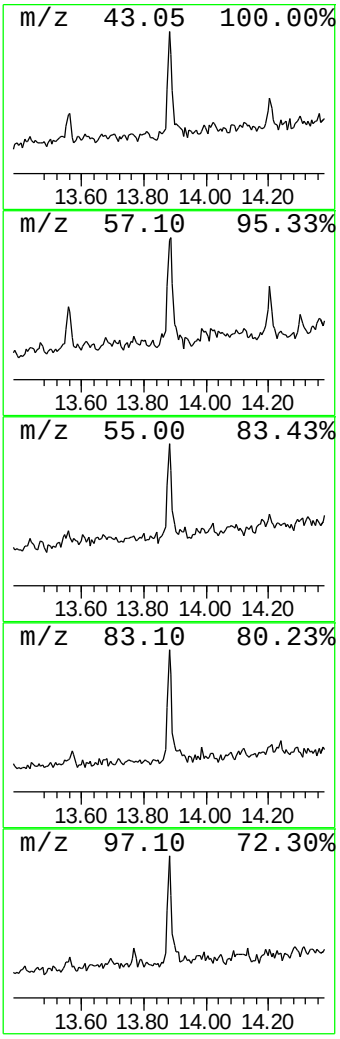
Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	4.03 ng	122589	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	81
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	76
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	76
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF111317\
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Misc :
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Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	12.2	ng	325658	1	6.89	532944	20.0
unknown6.66	6.66	68.7	ng	1830010	1	6.89	532944	20.0
Diethyltoluamide	10.30	3.6	ng	127933	3	9.93	707555	20.0
n-Hexadecanoic acid	11.93	7.1	ng	229344	4	11.41	645344	20.0
Pentadecanoic acid	12.71	2.6	ng	85232	4	11.41	645344	20.0
Octadecyl trifluo...	13.88	4.0	ng	122589	5	14.05	608496	20.0